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Use of the First Derivative of Spectral Reflectance to Detect Mold on Tomatoes

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ABSTRACT

THE first derivative of spectral reflectance of tomatoes was studied to see whether it can detect molds and sunscald damage on the fruit. The results indicate that a quality index based on the derivative values of reflectance at 590- and 710-nm wavelengths can be used to separate good tomates from those with black mold, gray mold, and sunscald.

INTRODUCTION

The presence of mold in harvested tomatoes affects fruit quality. The incidence of molds is high toward the end of the tomato-growing season. When the level of molding tomatoes exceeds 8 percent, the entire load can be rejected, resulting in economic loss.

Black mold is the most common of all tomato defects. It generally appears as black or dark brown spots on the surface of the fruit, although the infection may be underneath the skin, and the fruit has to be cut before the mold can be seen visually.

Although electro-optical sorters are being used commercially on harvesters to sort out green fruits and dirt clods, all other defects, including molds, must be sorted out by hand. When the incidence of molds is high, hand-sorters cannot handle the sorting. A high-speed electronic sorter would be more suitable for such sorting.

Researchers have investigated the use of reflectance measurement to detect mold and other defects on agricultural products. Moini et al. (1980) used reflectance at 670- and 960-nm wavelengths to detect molds and other defects on tomatoes. Surface defects on citrus fruits were studied by Gaffney (1973) and Felsenstein and Manor (1973). Brown et al. (1974) related near-infrared reflectance to bruises in apples. Other studies include detection of defects on radishes (Gaffney, 1976), surface damage on prunes (Burkhardt and Mrozek, 1973), and mold contamination in corn (Birth and Johnson, 1970).

In chemical analysis, the derivatives of absorbance spectrum are often used to help identify compound constituents in a solution, because of derivative spectra can aid greatly in defining the presence and locations of hidden absorption bands. Results of recent research on optical measurement of agricultural products indicate that, in quality evaluation of food, the analysis of the derivative spectra from spectral reflectance (or transmittance) can be more effective than the analysis of the reflectance itself (Norris and Barnes, 1976; Birth, 1979). Therefore, the derivative values of the spectral reflectance were used in this study to evaluate the presence of black mold and other defects on tomatoes.

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TABLE 1. QUALITY TYPES AND NUMBER OF FRUITS USED.

Quality type	Number tested	
	UV-VIS range	NIR range
Good	30	29
Black mold	66	48
Sunscald	5	14
Gray mold	12	13

OBJECTIVES

Objectives were to identify the wavelengths at which the first derivative values of the spectral reflectance correlate with the amount of black mold on tomatoes, and to establish criteria that can be used to separate moldy tomatoes from good ones.

EXPERIMENTAL PROCEDURE

A Perkin-Elmer model 340 double-beam recording spectrophotometer, equipped with an integrating sphere coated with magnesium-oxides, was used. Reflectance values were recorded as a percentage of the reference reflectance (magnesium-oxide slab) for both ultraviolet-visible (UV-VIS) and near-infrared (NIR) ranges.

Tomatoe samples were collected from a grading station in Woodland (California) and from field plots on the University of California Campus in Davis during September and October, 1979. Table 1 lists the number and quality types of the tomatoes tested. Emphasis was placed on the black mold because it presented a more critical problem than did other defects.

For spectral reflectance measurement, each tomato sample was placed in the spectrophotometer so that the area of interest was at the sample port of the integrating sphere. The monochromatic beam covers an area on the fruit surface of 5 mm square. After the sample was placed in the spectrophotometer, two consecutive scannings

TABLE 2. SPECTROPHOTOMETER SETTINGS USED TO RECORD THE REFLECTANCE AND FIRST DERIVATIVE CURVES.

	UV-VIS range	NIR range
Scanning speed, nm/min	220	500
Wavelength expansion, nm/cm	20	50
Slit width, nm	6	Auto-servo
Scale:		
Reflectance range	0 to 100%	0 to 100%
Derivative range	-30 to +30	-30 to +30
Wavelength increment ($\Delta\lambda$), nm (for determine derivative)	5	5

were made to trace the reflectance and the first derivative curves. Table 2 shows the spectrophotometer settings used.

The data for UV-VIS (190-850 nm) and NIR (850-2200 nm) ranges were taken separately because the integrating sphere had to be changed for each range. Therefore, the analysis of the data in these two ranges were performed separately.

The extent of mold damage in terms of both external and internal appearance was evaluated and coded with numerical values from 1 (least damage—a mold spot of 0.5 cm diameter and 0.2 cm deep) to 10 (worst damage—a mold spot that covers one-third the surface area of the fruit).

The reflectance and first derivative curves were plotted on a chart paper, and their numerical values at each 10-nm increment were printed out by an attached computerized data-handling unit. These numerical values were then punched on computer cards and transferred onto a disk file for further analysis.

ANALYSIS OF EXPERIMENTAL DATA

The reflectance value will be referred to as "R value" and the derivative value as "R′ value." The R and R′ values at wavelength λ_i will be denoted as R_{λ_i} and R'_{λ_i}, respectively.

The first part of the analysis was to select those wavelengths that show some correlation to the quality types. For computer identification purpose, a range of numerical values was assigned to each quality type: 100-199 for good red tomates, 200-399 for black molds, 400-599 for sunburns, 500-599 for sunscalds, and 600-699 for gray molds. A computer program was written to plot R′ vs. quality-type values for any given wavelength. Such a plot was made for each wavelength at 10-nm increments for the entire range. The criterion used to select the useful wavelengths for further analysis was based on the separation of the quality types in the plots. The wavelengths at which about two thirds of the points in the mold group were at a different level from those in the good tomato group were selected. This criterion was also applied to sunscalds and sunburns, although fewer data were available.

A number of wavelengths were selected that show possible correlation between R′ values and quality factors. Based on these selected wavelengths, two data matrices (one for the data in the UV-VIS range and one for those in the NIR range) were created and then analyzed using a stepwise discriminant analysis—a combination of analysis of variance, analysis of covariance, and multiple regression. A pre-written computer program, namely the P7M of the BMDP series (Dixon and Brown, 1979), was used to perform this analysis. This program performs a discriminant analysis between two or more groups. The variables used in computing the linear classification functions are chosen in a stepwise manner, both forward and backward. At each step, the variable that adds most to the separation of the groups is entered into (forward), or the variable that adds least is removed from (backward), the discriminant function. The computing process was described by Dixon and Brown (1979). The computer program computes a linear classification function based on the specified groups of tomatoes to be separated. This classification function can then be used as a quality index to classify the

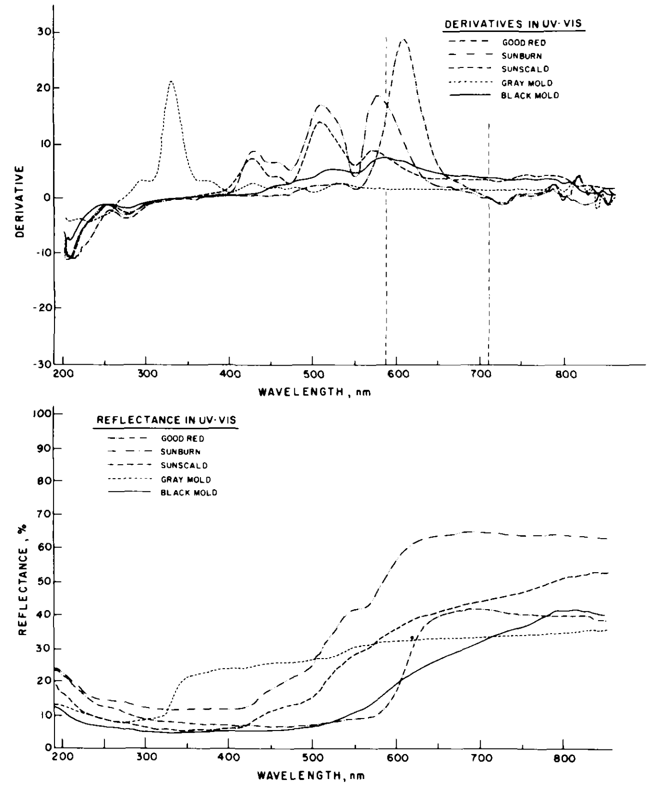

FIG. 1 Examples of first derivative curves (top) and spectral reflectance curves (bottom) for tomates in different quality types. UV-VIS range.

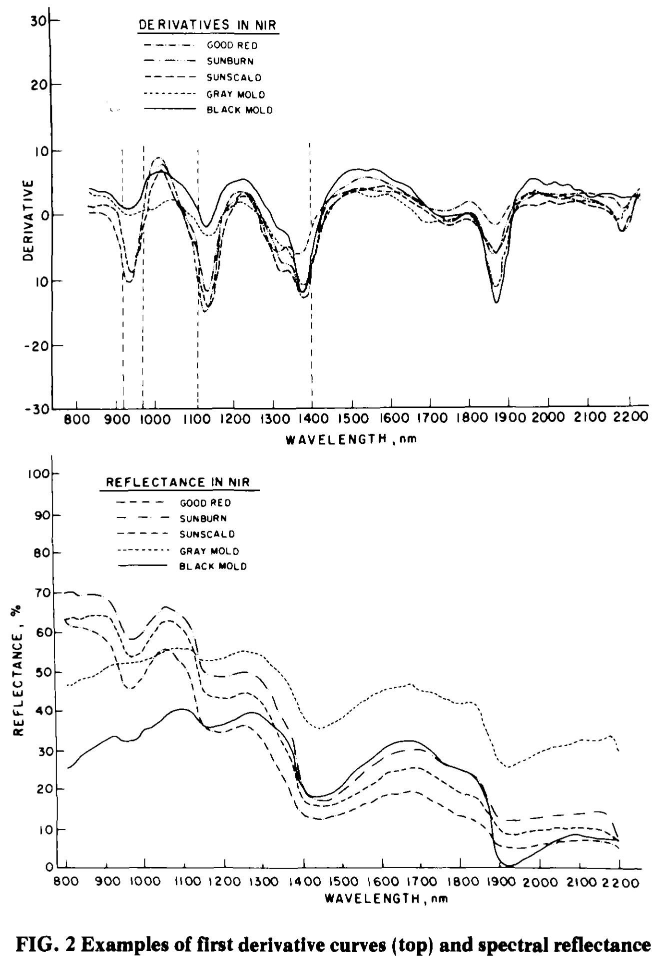

FIG. 2 Examples of first derivative curves (top) and spectral reflectance curves (bottom) for tomatoes in different quality types. NIR range.

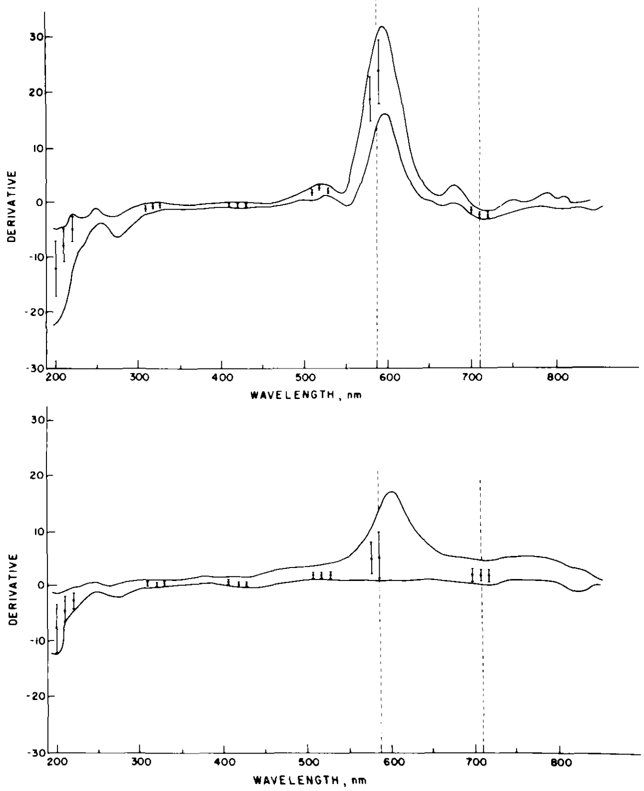

FIG. 3 The range of variation among the derivative curves for good tomatoes (top) and for black-mold tomatoes (bottom). UV-VIS range. Each bar represents the mean ± one standard deviation of the R′ value at each selected wavelength.

tomatoes by quality type.

The program also permits the selection of any variables (R_{λ_i}) and creation of new variables (combinations of R_{λ_i}) from existing ones by transformations (transformations performed by a computer subprogram which computes new variables as functions of other variables). Selected ratios of R′ values at two wavelengths and the averages of R′ values at three or more wavelengths were also analyzed, and the best linear discriminant function was obtained from them.

RESULTS AND DISCUSSION

Both the spectral reflectance curves and the spectral derivative curves show marked differences among tomatoes of different quality types. The differences are more pronounced in certain wavelength regions. Fig. 1 shows examples of the reflectance curves (bottom) and the derivative curves (top) in the UV-VIS range; Fig. 2 shows similar curves in the NIR range. The range of variation among the derivative cures for good tomatoes and for tomatoes with black mold are shown in Fig. 3 (for UV-VIS range) and Fig. 4 (for NIR range).

Computer plots of R′ values vs. quality-type values were made (one plot for each wavelength at 10-n, increments throughout the range). Seventeen wavelengths were selected in the UV-VIS range, and 31 wavelengths were selected in the NIR range. These wavelengths are listed by group in Table 3. Each group of neighboring wavelengths represents a band at which the R′ values among tomatoes of different quality types differ from one another. The R′ values at these wavelengths for all tomatoes tested were used in the stepwise discriminant analysis. Figs. 3 and 4 show the means and standard derivations of R′ values at these selected wavelengths for

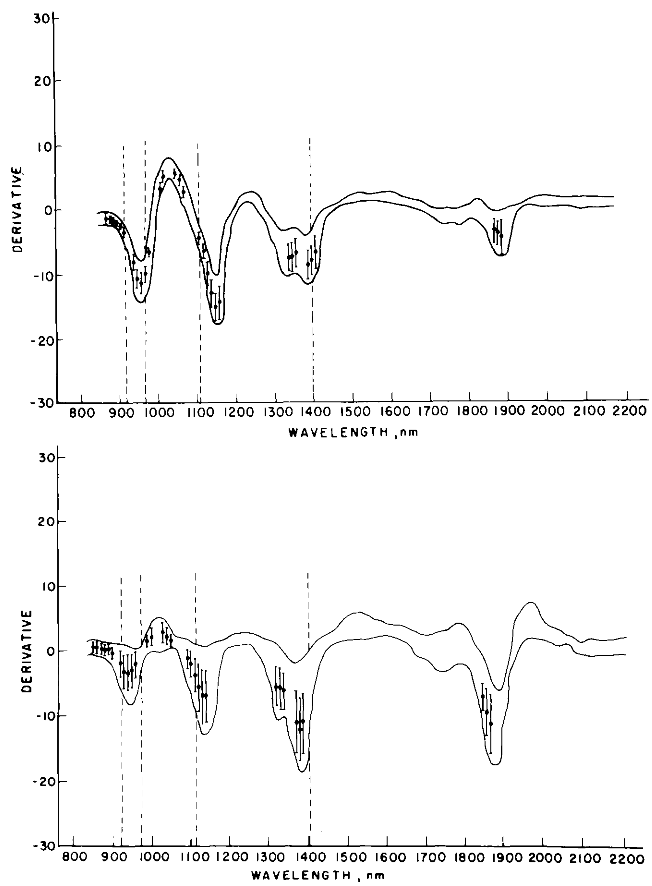

FIG. 4 The range of variation among the derivative curves for good tomatoes (top) and for black-mold tomatoes (bottom). NIR range. Each bar represents the mean ± one standard deviation of the R′ value at each selected wavelength.

good and moldy tomatoes.

Results of the stepwide discriminant analysis are summarized in Tables 4 and 5. The computation of the discriminant function in column 1 was based on the separation of the two quality types in column 2. The same discriminant function was then used to classify tomatoes in all quality types. The classification results are shown in column 3, 4, and 5. The numbers in these columns represent the percentage of correct classification for each group, and, in parenthesis, the group in which incorrectly classified fruits were placed. The mean value of the discriminant function of each group is shown in square brackets. The canonical correlation for each case is given in the last column.

The results indicate that the discriminant functions derived from R′ values in the UV-VIS range generally perform slightly better than those obtained from R′ values in the NIR range. The best discriminant function for separating black-mold and good tomatoes is ($0.18\ R'_{590} - 0.63\ R'_{710} - 1.73$). It classifies 100 percent of good

TABLE 3. LIST OF WAVELENGTHS SELECTED FOR STEPWISE DISCRIMINANT ANALYSIS.

UV-VIS range, nm	NIR range, nm
200, 210, 220	870, 880, 890, 900, 910, 920
310, 320, 330	940, 950, 960, 970, 980
410, 420, 430	1010, 1020
510, 520, 530	1050, 1060, 1070
580, 590	1110, 1120, 1130, 1140, 1150, 1160
700, 710, 720	1340, 1350, 1360
	1390, 1400, 1410
	1870, 1880, 1890

TABLE 4. COMPUTED DISCRIMINANT FUNCTIONS AND THE CLASSIFICATION RESULTS (UV-VIS RANGE).

Discriminiant function	Quality types to separate	Percentage of Correct classification* (incorrect type), [mean of function value] Good	Black Mold	Gray Mold	Sunscald	Canonical Correlation
$0.18\ R'_{590} - 0.63\ R'_{710} - 1.73$	Good - Black	100 [3.78]	98(good)† [-1.85]	(black) [-2.08]	(black) [-2.10]	0.937
$-0.008 \frac{R'_{600}}{R'_{420}} - 0.45 \frac{R'_{600}}{R'_{220}} - 1.67$	Good - Black	91 (black) [1.50]	91 (good) [-0.73]	(black) [-1.92]	(black) [-2.10]	0.728
$0.19\ R'_{220} - 2.12\ R'_{410} + 0.29\ R'_{580}$ $-209\ R'_{700} - 3.14$	Good - Gray	100 [4.35]	(gray, 96) (good, 4) [-6.40]	100 [-7.37]	(gray) [-20.64]	0.986
$-0.15\ R'_{510} + 0.21\ R'_{590}$ $-0.53\ R'_{710} - 1.36$	Good - Others	100 [4.33]	←	98 (good) [-1.56]	→	0.935

*See explanation below.

†98(good) [-1.85] means 98% of that quality type was correctly classified and the rest was incorrectly classified as good. The mean value of the determinant function for the group is [-1.85].

TABLE 5. COMPUTED DISCRIMINANT FUNCTIONS AND THE CLASSIFICATION RESULTS (NIR RANGE).

Discriminiant function	Quality types to separate	Percentage of correct classification (incorrect type), [mean of function value]* Good	Black Mold	Gray Mold	Sunscald	Canonical Correlation
$-0.81\ R'_{880} - 0.52\ R'_{1110} - 0.68$	Good - Black	100 [2.77]	94 (good)† [-1.33]	(black) [-1.38]	(black, 90) (good, 10) [-2.64]	0.890
$0.04 \frac{R'_{920}}{R'_{880}} - 0.76 \frac{R'_{1430}}{R'_{1360}}$ $- 3.66 \frac{R'_{1060}}{R'_{1400}} - 0.58$	Good - Black	96 (black) [1.55]	91 (good) [-0.76]	(black, 92) (good, 8) [-5.88]	(black) [-0.81]	0.740
$-1.15\ R'_{900} - 0.78\ R'_{970}$ $-0.14\ R'_{1400} - 6.86$	Good - Gray	100 [4.10]	(gray, 80) (good, 20) [-4.36]	100 [-7.51]	(gray, 80) (good, 20) [-6.51]	0.985
$-.30\ R'_{920} - 0.36\ R'_{950} + 0.47\ R'_{1390}$ $-0.36\ R'_{1400} - 0.62$	Good - Others	100 [3.12]	←	97 (good) [-0.97]	→	0.869

*See explanation below.

†94(good) [-1.33] means 98% of that quality type was correctly classified and the rest was incorrectly classified as good. The mean value of the determinant function for the group is [-1.33].

tomatoes and 98 percent of black-mold tomatoes correctly. The same function also classifies tomatoes with gray mold and sunscald tomatoes into the same category as those with black mold, indicating that the same functions can be used as a quality index to separate good tomatoes from those with any of the three types of defects with high accuracy.

Table 4 and 5 also include discriminant functions that wer computed on the basis of separation between good tomatoes and those with gray mold and between good tomatoes and those with any other defect. Although these functions may be suitable for classifying the two quality types used, none is better than the first function (in Table 4) in separating good tomatoes from those with black mold and other defects. The use of the ratios of two R'_{λ_i} as variables for computing the discriminant function did not improve the classification results.

CONCLUSIONS

The first derivative values of the spectral reflectance of tomatoes can be used to form a quality index for separating good tomatoes from those with black mold, gray mold, and sunscald. The best quality index is a linear combination of R′ values at 590- and 710-nm wavelengths in the following form: $0.18R'_{590} - 0.63\ R'_{710} - 1.73$.

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